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* * * * * Welcome to STN International * * * * *

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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the
present
NEWS 4 Jul 15 Data from 1960-1976 added to RDISCLOSURE
NEWS 5 Jul 21 Identification of STN records implemented
NEWS 6 Jul 21 Polymer class term count added to REGISTRY
NEWS 7 Jul 22 INPADOC: Basic index (/BI) enhanced; Simultaneous Left and
Right Truncation available
NEWS 8 AUG 05 New pricing for EUROPATFULL and PCTFULL effective
August 1, 2003
NEWS 9 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 10 AUG 15 PATDPAFULL: one FREE connect hour, per account, in
September 2003
NEWS 11 AUG 15 PCTGEN: one FREE connect hour, per account, in
September 2003
NEWS 12 AUG 15 RDISCLOSURE: one FREE connect hour, per account, in
September 2003
NEWS 13 AUG 15 TEMA: one FREE connect hour, per account, in
September 2003
NEWS 14 AUG 18 Data available for download as a PDF in RDISCLOSURE
NEWS 15 AUG 18 Simultaneous left and right truncation added to PASCAL
NEWS 16 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right
Truncation
NEWS 17 AUG 18 Simultaneous left and right truncation added to ANABSTR
NEWS 18 SEP 22 DIPPR file reloaded
NEWS 19 SEP 25 INPADOC: Legal Status data to be reloaded
NEWS 20 SEP 29 DISSABS now available on STN

NEWS EXPRESS OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
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NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 06:55:50 ON 09 OCT 2003

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 06:55:57 ON 09 OCT 2003

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STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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Uploading 10058456.str

L1 STRUCTURE UPLOADED

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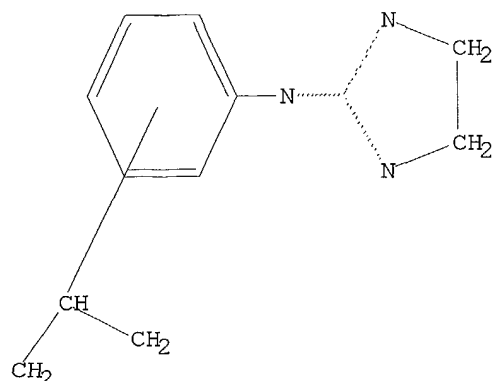
Uploading 10058456.str

L2 STRUCTURE UPLOADED

=> d

L2 HAS NO ANSWERS

L2 STR



G1 H,X,O,C

G2 C,H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l2 full

FULL SEARCH INITIATED 06:56:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 23843 TO ITERATE

100.0% PROCESSED 23843 ITERATIONS

23 ANSWERS

SEARCH TIME: 00.00.01

L3 23 SEA SSS FUL L2

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.15

148.36

FILE 'CAPLUS' ENTERED AT 06:56:50 ON 09 OCT 2003

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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15

FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

Page 4 10/09/2003

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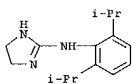
L4 18 L3

=> d ibib abs hitstr 1-18

L4 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2003:266866 CAPLUS
 DOCUMENT NUMBER: 139:96683
 TITLE: Inhibitors of calling behavior of *Plodia interpunctella*
 AUTHOR(S): Hirashima, Akinori; Shigeta, Yoko; Eiraku, Tomohiko; Kuwano, Eiichi
 CORPORATE SOURCE: Dep. Applied Genetics Pest Management, Fac. Agriculture, Grad. Sch., Kyushu Univ., Higashi-ku, Fukuoka, 812-8581, Japan
 SOURCE: Journal of Insect Science (Tucson, AZ, United States) (2003), 3, No pp. given
 CODEN: JISTCY; ISSN: 1536-2442
 URL: http://www.insectscience.org/3.4/Hirashima_et.al.
 JIS_3_4_2003.pdf
 PUBLISHER: University of Arizona Library
 DOCUMENT TYPE: Journal: (online computer file)
 LANGUAGE: English

AB Some octopamine agonists were found to suppress the calling behavior of the stored product Indian meal moth, *Plodia interpunctella*. Compds. were screened using a calling behavior bioassay using female *P. interpunctella*. Four active derivs., with inhibitory activity at the nanomolar range were identified in order to decreasing activity: 2-(1-phenylethylamino)-2-oxazoline > 2-(2-Et,6-methylanilino)oxazolidine > 2-(2-Me benzylamino)-2-thiazoline > 2-(2,6-diethylanilino)thiazolidine. Three-dimensional pharmacophore hypotheses were built from a set of 15 compds. Among the ten common-featured models generated by the program Catalyst/HipHop, a hypothesis including a hydrogen-bond acceptor lipid, a hydrophobic arom. and two hydrophobic aliph. features was considered to be essential for inhibitory activity in the calling behavior. Active compds. mapped well onto all the hydrogen-bond acceptor lipid, hydrophobic arom. and hydrophobic aliph. features of the hypothesis. On the other hand, less active compds. were shown not to achieve the energetically favorable conformation that is found in the active molts. in order to fit the 3D common-feature pharmacophore models. The present studies demonstrate that inhibition of calling behavior is via an octopamine receptor.

IT 63346-74-7 558484-41-6
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (Inhibitors of calling behavior of *Plodia interpunctella*)
 RN 63346-74-7 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

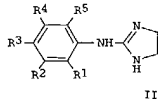
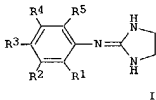


RN 558484-41-6 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2-ethyl-6-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:609547 CAPLUS
 DOCUMENT NUMBER: 137:169519
 TITLE: Preparation of new alkyl phenyl imino imidazolidine derivatives for treatment of urinary incontinence
 INVENTOR(S): Esser, Franz; Pouzet, Pascale; Arielle, Jane-Josée; Kitagawa, Hisator; Sakai, Kenji; Muramatsu, Ikunobu; Hoffmann, Matthias
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Kg, Germany
 SOURCE: Ger. Offen., 14 pp.
 CODEN: GWXXEX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

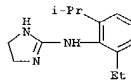
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10106214	A1	20020814	DE 2001-10106214	20010210
WO 2002064570	A1	20020822	WO 2002-EP576	20020122
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NC, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KK, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LB, MC, NI, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002169193 A1 20021114 US 2002-58456 20020128				
PRIORITY APPLN. INFO.: DE 2001-10106214 A 20010210 US 2001-270333P P 20010221				

OTHER SOURCE(S): MARPAT 137:169519
 GI



AB The present invention covers (m-alkylphenylimino)imidazolidine derivs. I [R1, R5 = H, F, Cl, Br, CF3, Me, OMe; R2, R4 = H, C3-6-alkyl; R3 = H, F, Cl, Br, CF3, Me], or its tautomers II and their pharmacol. acceptable salts, and their use for the prodn. of drugs, in particular for the treatment of urinary incontinence. Thus, I (R1 = R3 = R4 = H, R2 = CMe3, R5 = OMe) was prepd. from 5-(tert-butyl)-2-methoxyaniline via reaction with potassium isothiocyanate in acetone contg. PhCOCl followed by cyclocondensation with (CH2NH2)2 in MeOH contg. MeI. I (R1 = R3 = R4 = H, R2 = CMe3, R5 = OMe) was tested for its effectiveness [bioavailability = 34% in rat plasma; 0.7% deqrdn. in the presence of enzyme CYP2D6; 71% contraction in dogs vs. 30% contraction in human urethra].
 IT 446252-27-3P 446252-29-5P 446252-30-8P
 446252-31-9P, 2-[(6-Bromo-3-isopropyl)-2-

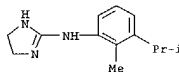
L4 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



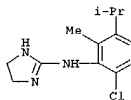
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

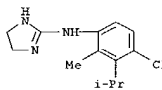
methylphenyl)imino]imidazolidine 446252-33-1P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (Prepn. of new alkyl Ph imino imidazolidine derivs. for treatment of urinary incontinence)
 RN 446252-27-3 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2-methyl-3-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



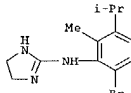
RN 446252-29-5 CAPLUS
 CN 1H-Imidazol-2-amine, N-[6-chloro-2-methyl-3-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



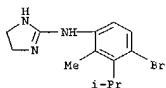
RN 446252-30-8 CAPLUS
 CN 1H-Imidazol-2-amine, N-[4-chloro-2-methyl-3-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 446252-31-9 CAPLUS
 CN 1H-Imidazol-2-amine, N-[6-bromo-2-methyl-3-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

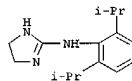


L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 RN 446252-33-1 CAPLUS
 CN 1H-Imidazol-2-amine, N-[4-bromo-2-methyl-3-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



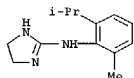
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:983550 CAPLUS
 DOCUMENT NUMBER: 136:320707
 TITLE: Three-Dimensional common-Feature hypotheses for octopamine agonist 2-(arylimino)imidazolidines
 AUTHOR(S): Hirashima, Akinori; Morimoto, Masako; Kuwano, Eiichi; Taniguchi, Eiichi; Eto, Morifusa
 CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Kyushu University, Faculty of Agriculture, Graduate School, Fukuoka, Higashi-ku, 812-8581, Japan
 SOURCE: Bioorganic & Medicinal Chemistry (2001), Volume Date 2002, 10(1), 117-123
 CODEN: BMCECF; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Three-dimensional pharmacophore hypotheses were built from a set of 10 octopamine (OA) agonist 2-(Arylimino)imidazolidines (AIIIs), 2-(Arylimino)thiazolidines (AITs) and 2-(Arylimino)oxazolidines (AIOs). OA agonist activities were detd. using the adenylate cyclase assay in American cockroaches (*P. americana*). Among the 10 common-featured models generated by program Catalyst/HipHop, a hypothesis including a ring arom. (RA), a pos. ionizable (PI) and three hydrophobic aliph. (HpAl) features was considered to be important in evaluating the OA-agonist activity. Active OA agonist 2,6-Et2 AII mapped well onto all the RA, PI and HpAl features of the hypothesis. On the other hand, less active compds. were shown to be difficult to achieve the energetically favorable conformation which is found in the active mols. in order to fit the 3-D common-feature pharmacophore models. Taken together, 2,6-Et2-Ph and foramidine structures are important as OA agonists. The present studies on OA agonists demonstrate that a RA, a PI and three HpAl sites located on the mol. seem to be essential for OA-agonist activity.
 IT 63346-74-7 359668-33-0
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (QSAR for octopamine agonist (arylimino)imidazolidines)
 RN 63346-74-7 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



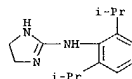
RN 359668-33-0 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



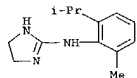
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:596828 CAPLUS
 DOCUMENT NUMBER: 135:222824
 TITLE: Identification of novel inhibitors of calling and in vitro [14C]acetate incorporation by pheromone glands of *Plodia interpunctella*
 AUTHOR(S): Hirashima, Akinori; Eiraku, Tomohiko; Watanabe, Yasuyuki; Kuwano, Eiichi; Taniguchi, Eiichi; Eto, Morifusa
 CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Faculty of Agriculture, Graduate School, Kyushu University, Fukuoka, 812-8581, Japan
 SOURCE: Pest Management Science (2001), 57(8), 713-720
 CODEN: PMSCF; ISSN: 1526-498X
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Some octopamine agonists were found to suppress in vitro biosynthesis of the calling pheromone of the Indian meal moth, *Plodia interpunctella*. Isolated pheromone-gland preps. incorporated sodium [14C]acetate at a linear rate for 3h when incubated with the pheromone biosynthesis activating neuropeptide (PBAN). This incorporation was dependent on the dose of PBAN (up to 0.5 μ M). Thin-layer chromatog. of a pheromone-gland ext. revealed quant. incorporation of radioactivity into a product exhibiting the same mobility as (Z,E)-9,12-tetradecadienyl acetate, the main component of the calling pheromone of *P. interpunctella*. Twenty-seven octopamine agonists were initially screened using a calling behavior bioassay of female *P. interpunctella*. Four derivs. with activity in the nanomolar range were identified which were, in order of decreasing pheromonostatic activity: 2-(2,6-diethylphenylimino)thiazolidine > 2-(2,6-dimethylphenylimino)thiazolidine > 2-(2-ethylphenylimino)oxazolidine. These compds. also showed in vitro inhibitory activity in intracellular de novo pheromone biosynthesis. The results of the present study indicate that these derivs. could provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.
 IT 63346-74-7P 359668-33-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prep. and pheromonostatic activity of)
 RN 63346-74-7 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 359668-33-0 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

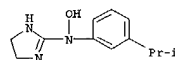
L4 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:37784 CAPLUS
DOCUMENT NUMBER: 134:231513
TITLE: Synthesis, structure, and binding of some 2-imidazolines to rat brain α -1 and α -2-adrenergic receptors
AUTHOR(S): Saczewski, F.; Kobierska, E.; Debowski, T.; Charskiewa-Minol, S.; Mokrosz, M.; Gdaniec, M.; Nowak, E.
CORPORATE SOURCE: Department of Chemical Technology of Drug and Organic Chemistry, Medical University of Gdansk, Pol.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(12), 425-430
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:231513
AB A series of novel 2-[(2-aminophenyl)imino]imidazolinium salts and N-benzyl-N-(4,5-dihydro-imidazol-2-yl)-O-methylhydroxylamine hydrochloride were prepd. and their structure was detd. by IR and NMR spectroscopic data as well as X-ray anal. of the imidazolinium azide salt of one of the compds. Binding evaluation for both α -1- and α -2-adrenergic receptors in rat brain preps. of these compds. and previously described α -1-hydroxy-2-aryliminoimidazolines 11a-d, N-(4,5-dihydroimidazol-2-yl)-1,3-2-oxodihydrobenzimidazoles, 2-amino-N-(4,5-dihydroimidazol-2-yl)-benzimidazoles, and N-(4,5-dihydroimidazol-2-yl)-indoles was performed. Among the compds. tested, 2-[(2-amino-4,5-dichlorophenyl)imino]imidazolinium chloride showed highest binding affinity to α -1- and α -2-adrenoreceptors ($K_i = 30$ nM).
IT 330685-57-9
RI: BFR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(synthesis, structure, and binding of imidazolines to brain α -1- and α -2-adrenergic receptors)
RN 330685-57-9 CAPLUS
CN 1H-imidazol-2-amine, 4,5-dihydro-N-hydroxy-N-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

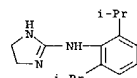


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L4 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN

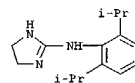
ACCESSION NUMBER: 2000:142505 CAPLUS
DOCUMENT NUMBER: 132:330832
TITLE: Three-dimensional molecular field analyses of octopaminergic agonists and antagonists for the locust neuronal octopamine receptor class 3
AUTHOR(S): Hirashima, A.; Nagata, T.; Fan, C.; Kuwano, E.; Taniguchi, E.; Eto, M.
CORPORATE SOURCE: Graduate School, Division of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, Japan
SOURCE: Journal of Molecular Graphics & Modelling (2000), Volume Date 1999, 17(3/4), 198-206
CODEN: JMGML; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The quant. structure-activity relationship (QSAR) of a set of 70 octopaminergic agonists and 20 antagonists against octopamine receptor class 3 (OAR3) in locust nervous tissue was analyzed by mol. field anal. (MFA). MFA of these compds. evaluated effectively the energy between a probe and a mol. model at a series of points defined by a rectangular grid. Contour surfaces for the mol. fields are presented. These results provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.
IT 63346-74-7
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(three-dimensional mol. field analyses of octopaminergic agonists and antagonists for locust neuronal octopamine receptor class 3)
RN 63346-74-7 CAPLUS
CN 1H-imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN

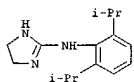
ACCESSION NUMBER: 2000:138409 CAPLUS
DOCUMENT NUMBER: 132:260196
TITLE: Prediction of distribution coefficients from structure. Comparison of calculated and experimental data for various drugs
AUTHOR(S): Tsantili-Kakoulidou, A.; Panderi, I.; Piperaki, S.; Cizmadi, F.; Darvas, F.
CORPORATE SOURCE: Department of Pharmacy, University of Athens, Athens, 157 01, Greece
SOURCE: European Journal of Drug Metabolism and Pharmacokinetics (1999), 24(3), 205-212
CODEN: EJDPD2; ISSN: 0378-7966
PUBLISHER: Medicine et Hygiene
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The efficiency of the program PrologD to predict distribution coeffs. (D) at any pH and pairing ion concn. has been tested using exptl. logD values for various drugs measured under std. conditions of buffers and ionic strength. Clonidine derivs., fluoroquinolones and β -blockers were included as particular pharmacol. classes within the testing data set. Calcns. were performed using the three logP estn. options implemented in the program. PrologD proved to be very efficient and can be of great advantage in drug research. Prediction patterns and correlations between exptl. and calcd. data indicate acceptable results for more than 80% of the data. In addn., comparable studies using the different options permitted suggestions for the more suitable logP estn. method in respect of the particular classes of compds.
IT 63346-74-7
RI: BFR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(comparison of calcd. and exptl. data for various drugs in prediction of distribution coeffs. from structure)
RN 63346-74-7 CAPLUS
CN 1H-imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



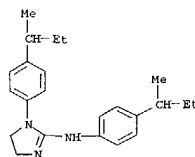
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:450898 CAPLUS
 DOCUMENT NUMBER: 129:175167
 TITLE: Design, Synthesis, and Pharmacological Evaluation of Conformationally Constrained Analogs of N,N'-Diaryl- and N-Aryl-N-alkylguanidines as Potent Inhibitors of Neuronal Na⁺ Channels
 AUTHOR(S): Maillard, Michel C.; Perlman, Michael E.; Amitay, Oved; Baxter, Deborah; Berlove, David; Connaughton, Sonia; Fischer, James E.; Guo, Jun Qing; Hu, Lian-Yen; McBurney, Robert N.; Nagy, Peter I.; Subbarao, Kataragadda; Yost, Elizabeth A.; Zhang, Lu; Durant, Graham J.
 CORPORATE SOURCE: Cambridge Neuroscience Inc., Cambridge, MA, 02139, USA
 SOURCE: Journal of Medicinal Chemistry (1998), 41(16), 3048-3061
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB In the present investigation, the rationale for the design, synthesis, and biol. evaluation of potent inhibitors of neuronal Na⁺ channels is described. N,N'-Diaryl- and N-aryl-N-alkylguanidine templates were locked in conformations mimicking the permissible conformations of the flexible diarylguanidinium ion (AS⁺, AA⁺, SS⁺). The resulting set of constrained guanidines termed "lockamers" (cyclophane, quinazoline, aminopyrimidazoles, aminimidazoles, azocino- and tetrahydroquinolinocarbonylguanidines) was examd. for neuronal Na⁺ channel blockade properties. Inhibition of [14C]guanidinium ion influx in CHO cells expressing type IIA Na⁺ channels showed that an aminopyrimidazoline deriv. and an aminimidazoline deriv., compds. proposed to lock the N,N'-diarylguanidinium in an SS⁺ conformation, were the most potent Na⁺ channel blockers with IC50's of 0.06 .mu.M. The rest of the restricted analogs with 4-p-alkyl substituents retained potency with IC50 values ranging between 0.46 and 2.9 .mu.M. Evaluation in a synaptosomal 45Ca2+ influx assay showed that the compds. did not exhibit high selectivity for neuronal Na⁺ vs Ca2+ channels. The retention of significant neuronal Na⁺ blockade in all types of semirigid conformers gives evidence for a multiple mode of binding in this class of compds. and can possibly be attributed to a poor structural specificity of the site(s) of action.
 IT 211558-28-0P
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. of conformationally constrained analogs of diaryl- and arylalkylguanidines as potent inhibitors of neuronal Na⁺ channels)
 RN 211558-28-0 CAPLUS
 CN 1H-imidazol-2-amine, 4,5-dihydro-N,1-bis[4-(1-methylpropyl)phenyl]-, monomethanesulfonate (9CI) (CA INDEX NAME)
 CM 1
 CRN 211558-27-9
 CMF C23 H31 N3

L4 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1997:669819 CAPLUS
 DOCUMENT NUMBER: 127:274156
 TITLE: Neurotransmitter-receptors as targets for new insecticides
 AUTHOR(S): Roeder, T.; Degen, J.; Dyczkowski, C.; Gewecke, M.
 CORPORATE SOURCE: Zoologisches Institut, Universität Hamburg, Neurophysiologie, Hamburg, D-20146, Germany
 SOURCE: New Strategies in Locust Control (1997), 219-223.
 Editor(s): Krall, S.; Feveling, R.; Ba Diallo, D.
 Birkhäuser: Basel, Switz.
 CODEN: 65BDA4
 CONFERENCE
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB The locust neuronal octopamine receptor is believed to be an ideal target for highly specific insecticides. The authors characterized a no. of high affinity agonists of this receptor subtype. Using structure-activity relationships, the authors were able to optimize the structure of these compds. in terms of their affinities. A variety of these compds. show a high degree of specificity for insect octopamine receptors vs. vertebrate adrenergic receptors. The high affinity together with the high degree of specificity makes compds. such as the phenyliminoimidazolidines ideal starting points for the development of new insecticides.
 IT 63346-74-7, NC 20
 RI: BSU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
 (affinity for locust neuronal octopamine receptor)
 RN 63346-74-7 CAPLUS
 CN 1H-imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



CM 2
 CRN 75-75-2
 CMF C H4 O3 S



REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1997:594632 CAPLUS
 DOCUMENT NUMBER: 127:262678
 TITLE: Preparation of novel indoles and benzothiazoles for cloned human alpha 2 receptors
 INVENTOR(S): Jeon, Yoon T.; Gluchowski, Charles
 PATENT ASSIGNER(S): Synaptic Pharmaceutical Corp., USA
 SOURCE: PCT Int. Appl., 73 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

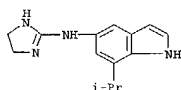
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731636	A1	19970904	WO 1997-US3173	19970228
W:	AL, AM, AT, AU, AZ, BA, BE, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH			
RW:	GH, KE, LS, MW, SD, SE, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
US 5677321	A	19971014	US 1996-608598	19960229
CA 2246813	AA	19970904	CA 1997-2246813	19970228
AU 9720604	A1	19970916	AU 1997-20604	19970228
AU 704439	B2	19990422		
EP 900080	A1	19990310	EP 1997-908782	19970228
R:	AT, BE, CH, DE, DK, ES, FR, GE, GR, IT, LT, LU, NL, SE, MC, PT, IE, FI			
JP 2000506144	T2	20000523	JP 1997-531156	19970228
US 5948804	A	19990907	US 1997-926316	19970905
US 6040451	A	20000321	US 1999-345470	19990630
US 6159998	A	20001212	US 2000-492505	20000127
US 6303643	B1	20011016	US 2000-690620	20001017
US 2002049239	A1	20020425	US 2001-965944	20010928
US 6498177	B2	20021224		
US 2003105147	A1	20030605	US 2002-278608	20021022
PRIORITY APPL. INFO.:			US 1996-608598	A 19960229
			WO 1997-US3173	W 19970228
			US 1997-926316	A1 19970905
			US 1999-345470	A1 19990630
			US 2000-492505	A1 20000127
			US 2000-690620	A1 20001017
			US 2001-965944	A1 20010928

OTHER SOURCE(S): MARPAT 127:262678
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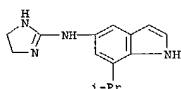
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I-IV; R1-R3 = H, C1-7 alkyl, C2-7 alkenyl, alkynyl; R4-R6 = H, halo, Oh, etc.; R7 = H, NH, C1-7 alkyl, etc.; R8 = H, C1-7 alkyl, C2-7 alkenyl, etc.; R9 = H, Ph, C1-7 alkyl, etc.; X = CH2, O, NH, S] which are selective for cloned human alpha 2 receptors and therefore useful for lowering intraocular pressure, for treating presbyopia, migraine, hypertension, alc. withdrawal, drug addiction, rheumatoid

L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 arthritis, ischemic pain, spasticity, diarrhea, nasal congestion, urinary incontinence as well as for use as analgesics, sedatives, anesthetics, cognition enhancers and ocular vasoconstriction agents, were prepd. Thus, reaction of 7-bromo-5-aminindole with 2-imidazoline-2-sulfonic acid (ISA) afforded 46% I [R1-R5 = H; R6 = Br; R7-R9 = H; X = N] which showed pEC50 of 9.36 at alpha 2 receptor.
 IT 196204-74-7P 196204-75-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of novel indoles and benzothiazoles for cloned human alpha 2 receptors)
 RN 196204-74-7 CAPLUS
 CN 1H-indol-5-amine, N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)- (9CI) (CA INDEX NAME)



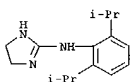
RN 196204-75-8 CAPLUS
 CN Butanedioic acid, compd. with N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)-1H-indol-5-amine (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 196204-74-7
 CMP C14 H18 N4



CM 2
 CRN 110-15-6
 CMP C4 H6 O4

HO2C--CH2--CH2--CO2H

L4 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1995:303934 CAPLUS
 DOCUMENT NUMBER: 122:77274
 TITLE: Pharmacology of the octopamine receptor from locust central nervous tissue (OAR3)
 AUTHOR(S): Roeder, Thomas
 CORPORATE SOURCE: Zool. Inst., Univ. Hamburg, Hamburg, D-20146, Germany
 SOURCE: British Journal of Pharmacology (1995), 114(1), 210-16
 CODEN: BJPCRM; ISSN: 0007-1188
 PUBLISHER: Stockton
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The present study characterized highly effective agonists from different classes of compds. for the neuronal octopamine receptor (OAR3) of the migratory locust (*Locusta migratoria* L.). Biogenic amines and phenyliminoimidazolidines (PIIs) were employed for the study of structure-activity relationships. The highest affinity PIIs were predominantly those with the substitutions at the positions 2 and 4 of the phenolic ring (e.g. NC 7, KI = 0.3 nM, NC8, KI = 0.81 nM). Substitutions at these positions always had pos. effects on the affinity of the resp. agonists. Substitutions at the positions 3, 5 and 6, however, always had neg. effects on the affinity. At the position one of the phenolic ring, heterocyclic substituents are preferred. Some PIIs had a more than 30 times higher affinity for OARs than for .alpha.-adrenoceptors which are the vertebrate homologues of the insect octopamine receptors. The only non-PIL with subnanomolar affinity was the aminooxazoline deriv. AC 6 (KI = 0.92 nM). A variety of substances with known insecticidal activity such as chlordaneform, demethylchlordaneform, amitraz or AC 6 had high affinity for the locust neuronal octopamine receptor.
 IT 63346-74-7, NC 20
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); FRP (Properties); BIOL (Biological study)
 (structure-activity relationship of agonists for locust neuronal octopamine receptor)
 RN 63346-74-7 CAPLUS
 CN 1H-imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

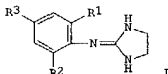


L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

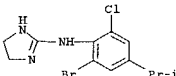
L4 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1989:95240 CAPLUS
 DOCUMENT NUMBER: 110:95240
 TITLE: Preparation of 2-(phenylimino)imidazolidines as .alpha.-1-adrenergic agonists
 INVENTOR(S): Esser, Franz; Staehle, Helmut; Kneppa, Herbert; Speck, Georg; Mierau, Joachim; Pichler, Ludwig; Lehr, Erich
 PATENT ASSIGNEE(S): Boehringer Ingelheim K.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 7 pp.
 CODEN: GWXXEX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3712385	A1	19881027	DE 1987-3712385	19870411
PRIORITY APPLN. INFO.:		DE 1987-3712385 19870411		
OTHER SOURCE(S):		CASREACT 110:95240; MARPAT 110:95240		

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AB The title compds. [I: R1, R2 = F, Cl, Br, iodo; R3 = (substituted) C1-4 alkyl] and pharmaceutically acceptable salts were prepd. as CNS agents and cyto- and cardioprotectants. KSCN in acetone was treated with PhCOCl at 15.degree. and 2-chloro-4-isopropylaniline was added. The mixt. was refluxed 3.25 h to give 70.5% (2-chloro-4-isopropylphenyl)thiourea. The latter was sequentially refluxed with MeI in MeOH, refluxed with H2NCH2CH2NH2 in MeOH, stirred with 5N NaOH, and treated with Br in CHCl3 at 0-8.degree. to give 2-(2-chloro-4-isopropylphenyl)imidazolidine.HBr. The latter at 1 mg/kg in mice increased survival in a hypoxia screen from 40% (controls) to 70%.
 IT 118955-15-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as CNS agent and cardio- and cytoprotectant)
 RN 118955-15-0 CAPLUS
 CN 1H-imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)



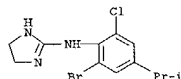
• HBr

L4 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

IT 118854-98-1P
 RL: SYN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as CNS agent, cyto- and cardioprotectant)

RN 118854-98-1 CAPLUS

CN 1H-Imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:593431 CAPLUS

DOCUMENT NUMBER: 103:193431

TITLE: Phenyliminoimidazolidines. Characterization of a class of potent agonists of octopamine-sensitive adenylate cyclase and their use in understanding the pharmacology of octopamine receptors

AUTHOR(S): Nathanson, James A.

CORPORATE SOURCE: Dep. Neurol., Harvard Med. Sch., Boston, MA, 02114, USA

SOURCE: Molecular Pharmacology (1985), 28(3), 254-68

CODEN: MOPMA3; ISSN: 0026-895X

DOCUMENT TYPE: Journal

LANGUAGE: English

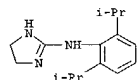
AB Approx. 30 substituted phenyliminoimidazolidines (PII) were examd. for agonist and antagonist effects on the highly enriched and specific octopamine (O)-sensitive adenylate cyclase (AC) present in the firefly light organ, as well as on ACs present in other invertebrate and vertebrate tissues. Several derivs. were extremely active and some had potencies exceeding those of any previously described agonists of O-sensitive AC. Stimulation by the potent PIIs was reversible, nonadditive to that caused by O, and could be antagonized by antagonists such as cyproheptadine, phenolamine, and propranolol. The inhibitory consts. agreed well with those for inhibiting O stimulation. Certain PII derivs. acted as partial agonists and some as antagonists of O stimulation. Structure-activity relationships revealed, among other things, that short-chain alkyl substitution in the 2- and 6-Phe positions enhanced activity, as did further substitution of 4-halo, 4-Me, or 4-hydroxy substituents. 4-Amino or N-alkyl substitution decreased activity. Structurally related benzylimidazoline derivs. such as tolazoline and naphazoline were partial O agonists, generally less active than the PIIs. Comparison, in 3 invertebrate species, of the effects of the PIIs and 2 other chem. classes of O agonists demonstrated clearcut differences in species responsiveness. Other comparative studies revealed that the agonist activity of the potent PIIs was specific for tissues contg. an O-sensitive AC; ACs activated by dopamine or by .beta.1- or .beta.2-adrenergic agonists were unaffected by these compds. The active PIIs affected a class of O receptors distinct from mammalian .alpha.1- or .alpha.2-adrenergic receptors. These O receptors also appeared distinct from mammalian 5-HT1 and 5-HT2 receptors. Correlative physiol. studies in insects revealed that the active PIIs mimicked O and were potent activators of light emission in the firefly light organ. The PIIs also cause disruption of motor and feeding behavior in tobacco hornworms, leading to insect death, an effect which was markedly potentiated by phosphodiesterase inhibitors.

IT 63346-74-7
 RL: BIOL (Biological study)
 (octopamine-sensitive adenylate cyclase activation by, in light organ of firefly, structure in relation to)

RN 63346-74-7 CAPLUS

CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1982:455809 CAPLUS

DOCUMENT NUMBER: 97:55809

TITLE: Imidazole derivatives and their therapeutic use

INVENTOR(S): Ramuz, Henri

PATENT ASSIGNEE(S): Hoffmann-La Roche, F., et Cie. S. A., Switz.

SOURCE: Fr. Demande, 49 pp.

CODEN: FROXEL

DOCUMENT TYPE: Patent

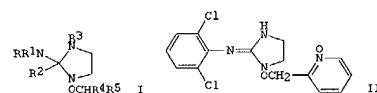
LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

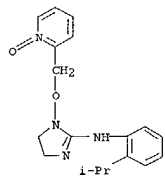
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2489822	A1	19820312	FR 1981-16998	19810908
CA 1175434	A1	19841002	CA 1981-383138	19810804
NL 8103721	A	19820401	NL 1981-3721	19810806
US 4366160	A	19821228	US 1981-296596	19810826
HU 28802	O	19831228	HU 1981-2529	19810902
EP 48363	A2	19820331	EP 1981-106900	19810903
EP 48363	A3	19820526		
EP 48363	B1	19850731		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3134956	A1	19820415	DE 1981-3134956	19810903
ZA 8106133	A	19820929	ZA 1981-6133	19810903
AT 14580	E	19850815	AT 1981-106900	19810903
SE 8105297	A	19820311	SE 1981-5297	19810907
FI 8102756	A	19820311	FI 1981-2756	19810907
DK 8103935	A	19820311	DK 1981-3935	19810907
AU 8175042	A1	19820318	AU 1981-75042	19810908
NO 8103074	A	19820311	NO 1981-3074	19810909
GB 2083475	A	19820324	GB 1981-27225	19810909
JP 57080382	A2	19820519	JP 1981-141135	19810909
BR 8105751	A	19820525	BR 1981-5751	19810909
ES 505322	A1	19820816	ES 1981-505322	19810909
ES 510795	A1	19830601	ES 1982-510795	19820325
PRIORITY APPLN. INFO.:			CH 1980-6798	19800910
			CH 1981-4175	19810624
			EP 1981-106900	19810903

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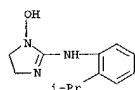


AB Imidazoles I [R = (un)substituted Ph; R1 = alkyl, alkenyl, aralkyl; R1R2, R2R3 = bond; R3 = H, alkyl, alkenyl, aralkyl, acyl; R4 = H, alkyl; R5 = (un)substituted pyridyl 1-oxide] were prepd. Thus 2-(2,6-dichlorophenylimino)imidazolidin-1-ol was treated with 2-chloromethylpyridine 1-oxide to give II which had an analgesic ED50 of 3.5 mg/kg orally in mice.

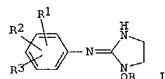
L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 IT 82401-27-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 82401-27-2 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-(1-methylethyl)phenyl]-1-[(1-oxido-2-pyridinyl)methoxy]- (9CI) (CA INDEX NAME)



IT 82401-26-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chloromethylpyridine oxide)
 RN 82401-26-1 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-1-hydroxy-N-[2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

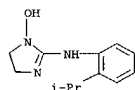


L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



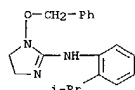
AB The iminoimidazolidines I (R = H, aryl, (cyclo) aliph. group optionally substituted by (alkylated) NH₂, CO₂H, or derivs., OH, CN, aryl, CONH₂, alkoxy, alkylthio, (substituted) pyridyl, etc.; R₁, R₂, R₃ = H, alkyl, alkoxy, alkylthio, halogen, CN, OH) and their salts were prepd. by 9 methods for use as antihypertensives and sympatholytics (test data tabulated). Thus, PhCH₂NHCH₂CH₂NH₂ reacted with 2,6-Cl₂C₆H₃N:CCl₂ to give I (R = PhCH₂, R₁ = 2-Cl, R₂ = 6-Cl R₃ = H), which was heated with 48% aq. HBr to give I (R = H).

IT 70923-38-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and O-acylation of)
 RN 70923-38-5 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-1-hydroxy-N-[2-(1-methylethyl)phenyl]-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

IT 70923-23-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 70923-23-8 CAPLUS
 CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-(1-methylethyl)phenyl]-1-(phenylmethoxy)- (9CI) (CA INDEX NAME)

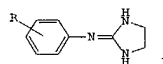


L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1979:611411 CAPLUS
 DOCUMENT NUMBER: 91:21141
 TITLE: 2-iminoimidazolidine derivatives
 INVENTOR(S): Ramuz, Henri
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
 SOURCE: Ger. Offen., 83 pp.
 CODEN: GWXXEX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2847766	A1	19790510	DE 1978-2847766	19781103
ZA 7806136	A	19791031	ZA 1978-6136	19781031
FR 2407919	A1	19790601	FR 1978-31026	19781102
AU 7841324	A1	19790517	AU 1978-41324	19781103
EP 2010	A1	19790530	EP 1978-101299	19781103
EP 2010	B1	19820714		
R: BE, CH, DE, FR, GB, LU, NL, SE				
DD 139847	C	19800123	DD 1978-208873	19781103
RO 76151	P	19810830	RO 1978-95588	19781103
CS 212309	P	19820326	CS 1978-7188	19781103
SU 831073	A3	19810515	SU 1978-2680652	19781104
NO 7803719	A	19790508	NO 1978-3719	19781106
DK 7804949	A	19790508	DK 1978-4949	19781106
GB 2008579	A	19790606	GB 1978-43271	19781106
GB 2008579	B2	19821103		
JP 54073779	A2	19790613	JP 1978-135936	19781106
SE 7811455	A	19790702	SE 1978-11455	19781106
US 4244957	A	19810113	US 1978-958300	19781106
CA 1106847	A1	19810811	CA 1978-315866	19781106
GB 2086379	A	19820512	GB 1979-81257	19781106
GB 2086379	B2	19821110		
AT 7807913	A	19821015	AT 1978-7913	19781106
AT 371112	B	19830610		
FI 7803393	A	19790508	FI 1978-3393	19781107
NL 7811070	A	19790509	NL 1978-11070	19781107
BR 7807317	A	19790724	BR 1978-7317	19781107
ES 480111	A1	19800401	ES 1979-480111	19790430
ES 480112	A1	19800401	ES 1979-480112	19790430
ES 480113	A1	19800401	ES 1979-480113	19790430
SU 910119	A3	19820228	SU 1979-2806102	19790831
CS 212310	P	19820326	CS 1980-2609	19800415
CS 212311	P	19820326	CS 1980-2610	19800415
US 4355033	A	19821019	US 1980-178223	19800814
US 4511720	A	19850416	US 1982-405476	19820805
PRIORITY APPLN. INFO.:			LU 1977-78467	19771107
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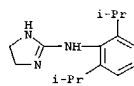
GI

L4 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1977:447931 CAPLUS
 DOCUMENT NUMBER: 87:47931
 TITLE: Structure-activity relations and problems related to the mechanism of action of clonidine
 AUTHOR(S): Roudot, Brunor; Leclerc, Gerard; Wermuth, Camille-Georges; Miesch, Francois; Schwartz, Jean
 CORPORATE SOURCE: Fac. Pharm., Univ. Louis-Pasteur, Strasbourg, Fr.
 SOURCE: Journal de Pharmacologie (1977), 8(1), 95-106
 CODEN: JNPHAG; ISSN: 0021-793X
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI

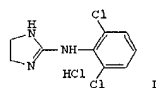


AB All 26 clonidine analogs (I) studied showed peripheral .alpha.-sympathomimetic activity, with IP₅₀ 56 (I; R = 2,3-dichloro) [15327-44-3] having the greatest hypertensive effect in desanguinated rats. The results correlated with E_s (steric const.) and F (sum of the field effect of the substituents) of the Hansch equation (1971). No such correlation was obsd. for hypotensive activity in intact rats. Compds. which had hypotensive activity also had high .alpha.-sympathomimetic activity, local anesthetic activity (rabbit cornea), and similar lipophilicity. However, the results were not sufficient to conclude that .alpha.-adrenergic mechanisms are involved in the hypotensive effects of clonidine and its analogs.

IT 63346-74-7
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (hypotensive and .alpha.-sympathomimetic activity of)
 RN 63346-74-7 CAPLUS
 CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



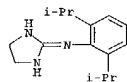
L4 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1976:456532 CAPLUS
 DOCUMENT NUMBER: 85:56532
 TITLE: Clonidine and related analogues. Quantitative correlations
 AUTHOR(S): Rouot, Bruno; Leclerc, Gerard; Wermuth, Camille G.; Miesch, Francois; Schwartz, Jean
 CORPORATE SOURCE: Fac. Pharm., Univ. Louis Pasteur, Strasbourg, Fr.
 SOURCE: Journal of Medicinal Chemistry (1976), 19(8), 1049-54
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A series of 22 derivs. of clonidine-HCl (I) [4205-91-8] were prepd. by the cyclization reaction of ethylenediamine with an S-methylisothiuronium salt deriv. and the main physicochem. parameters (log P, .DELTA.RM, pKa) detd. Quant. correlations between peripheral .alpha.-mimetic action (pithed rats) and physicochem. parameters pointed out the crit. role of the steric effect of ortho substituents. Attempted quant. correlations between physicochem. parameters and central hypotensive activity were unsuccessful. The mechanism of action of I is discussed.

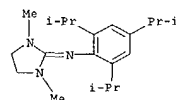
IT 59465-43-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and blood pressure response to)

RN 59465-43-9 CAPLUS
 CN Benzenamine, N-(1,3-dimethyl-2-imidazolidinylidene)-2,6-bis(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1975:592056 CAPLUS
 DOCUMENT NUMBER: 83:192056
 TITLE: Determination of the angle of twist in aryl compounds by carbon-13 nuclear magnetic resonance spectroscopy
 AUTHOR(S): Leibfritz, Dieter
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Frankfurt, Frankfurt/Main, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1975), 108(9), 3014-24
 CODEN: CHEBER; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA issue.
 AB The ¹³C NMR signal of the carbonyl C atom in benzoyl derivs. (e.g., I, R = H, Me, Me2CH, Me3C; R1 = Et, MeO, Cl, Me2N) moves to lower fields with increasing steric hindrance by ortho substituents, while the signal of the amino C in guanidines (e.g., II, R = H, Me, Me2CH) and imidazolidines (e.g., III, R = H, Me2CH) shifts to higher fields. The angle of twist can be calcd. from ¹³C NMR.
 IT 57199-06-1
 RL: PREP (Properties)
 (carbon-13 NMR of)
 RN 57199-06-1 CAPLUS
 CN Benzenamine, N-(1,3-dimethyl-2-imidazolidinylidene)-2,4,6-tris(1-methylethyl)- (9CI) (CA INDEX NAME)



=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

85.40

233.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-11.72

FILE 'REGISTRY' ENTERED AT 07:01:56 ON 09 OCT 2003

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STRUCTURE FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

DICTIONARY FILE UPDATES: 7 OCT 2003 HIGHEST RN 600637-01-2

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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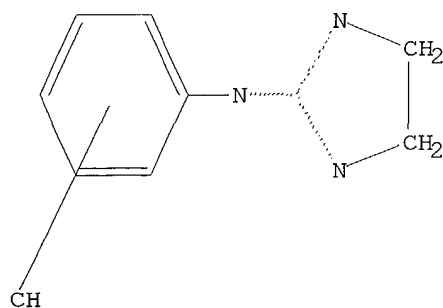
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L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR



G1 H, X, O, C

G2 C, H, X

Structure attributes must be viewed using STN Express query preparation.

=> s 15 full

FULL SEARCH INITIATED 07:02:16 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 23843 TO ITERATE

100.0% PROCESSED 23843 ITERATIONS

1145 ANSWERS

SEARCH TIME: 00.00.01

L6 1145 SEA SSS FUL L5

=> fil caplus

COST IN U.S. DOLLARS

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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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FILE COVERS 1907 - 9 Oct 2003 VOL 139 ISS 15

FILE LAST UPDATED: 8 Oct 2003 (20031008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L7 621 L6

=> d his

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FILE 'REGISTRY' ENTERED AT 06:55:57 ON 09 OCT 2003

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 23 S L2 FULL

FILE 'CAPLUS' ENTERED AT 06:56:50 ON 09 OCT 2003

L4 18 S L3

FILE 'REGISTRY' ENTERED AT 07:01:56 ON 09 OCT 2003

L5 STRUCTURE UPLOADED

L6 1145 S L5 FULL

FILE 'CAPLUS' ENTERED AT 07:02:20 ON 09 OCT 2003

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621 L6

L8 603 L6 NOT L4

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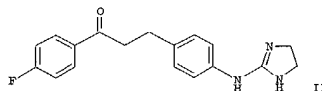
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, HU, IE, IL, IN, IT, JP, KE, KP, KR, KZ, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RU, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, VU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2002021808	A5	20020527	AU 2002-21808	20011105
BR 2001015291	A	20020819	BR 2001-15291	20011105
EP 1339694	A1	20030903	EP 2001-996531	20011105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 6417186	B1	20020709	US 2001-14110	20011113
US 2002091147	A1	20020711		
NO 2003002112	A	20030513	NO 2003-2142	20030513
PRIORITY CLAIMING INFO.:				
			US 2000-248888R	P 20001114
			WO 2001-EP12776	W 20011105
OTHER SOURCE(S):				
MARPAT 136:396115				
GI				

19 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)
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yl]propan-1-one 427897-01-6P, 3-[4-(4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-(4-
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1-[4-(4,5-dihydro-1H-imidazol-2-ylamino]phenyl]-1-[2,3,4-trichlorophenyl]propan-1-one hydrochloride 427897-17-4P,
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RL: PAC (Pharmacological activity) | SYN (Synthetic preparation) | THU (Therapeutic use) | BIOL (Biological study) | PREP (Preparation) | USES (Uses)

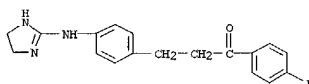
(drug substituted 2-phenylaminoimidazole) Pb ketone deriv. as human

R1-A-c1ccc(cc1)Nc2cc[nH]2

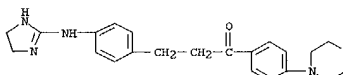
AB Title compds. 1 [1] were prepd. For instance, 4-fluorocetophenone and 4-nitrobenzaldehyde were reacted together (EtOAc, KOH) to give 1-[4-(fluorophenyl)-3-[4-(nitrophenyl)]propanone. This intermediate was reduced (EtOAc, H2-10% Pd/C) and reacted with 2-chloro-4,5-dihydro-1H-imidazole sulfate to give 1 in 54.2% overall yield. Example compds. had pKa's in the range 4.5-10.5, and the rate of action on receptors: if had pKa's = 9.50, 1 are used for the treatment of diseases assocd. with pain, inflammation, urinary tract disease states, respiratory disease states, edema formation, or hypotensive vascular diseases.

IT 427896-68-2P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-(fluorophenyl)]propan-1-one 427896-69-3P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-morpholin-4-ylphenyl]propan-1-one 427896-71-7P 427896-73-9P 427896-74-0P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-[4-(methanesulfonyl)piperazin-1-yl]phenyl]propan-1-one 427896-75-1P 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-[4-(furan-2-carbonyl)piperazin-1-yl]phenyl]propan-1-one 427896-76-2P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-isopropoxyphenyl]propan-1-one 427896-77-3P, 1-[2,4-Difluorophenyl]-3-[4-[4,5-dihydro-1H-imidazol-2-ylamino]phenyl]propan-1-one 427896-78-4P, 4-[4-[3-[4,5-dihydro-1H-imidazol-2-ylamino]phenyl]-1-fluoro-1-phenylethyl]butyric acid ethyl ester 427896-79-5P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[2-Fluoro-4-[morpholin-4-yl]phenyl]propan-1-one 427896-80-8P 427896-81-9P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-[4-methylpiperazin-1-yl]phenyl]propan-1-one 427896-82-0P 427896-83-1P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]propan-1-one 427896-83-1P, 1-[4-Chlorophenyl]-3-[4-[4,5-dihydro-1H-imidazol-2-ylamino]phenyl]propan-1-one 427896-94-2P, 1-[2,4-Dichlorophenyl]-3-[4-[4,5-dihydro-1H-imidazol-2-ylamino]phenyl]propan-1-one 427896-85-3P, 3-[4-[4,5-Dihydro-1H-imidazol-2-ylamino]phenyl]-1-[4-(phenylthio)phenyl]propan-1-one 427896-86-4P 427896-87-5P, 3-[4-[4,5-Dihydro-1H-

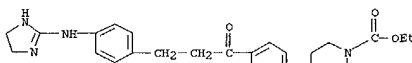
RN 427896-68-2 CAPLUS
 CN 1-Propanone, 3-(4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl)-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



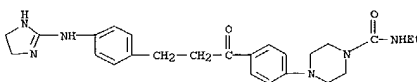
RN 427896-69-3 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 427896-71-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

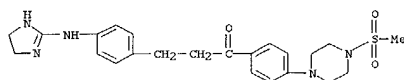


RN 427896-73-9 CAPLUS
CN 1-Piperazinecarboxamide, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)aminophenyl]-1-oxopropyl]phenyl]-N-ethyl]- (9CI) (CA INDEX NAME)

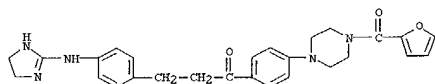


RN 427896-74-0 CAPLUS
CN Piperazine, 1-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

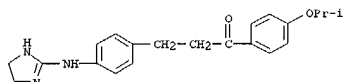
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



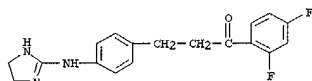
RN 427896-75-1 CAPLUS
CN Piperazine, 1-[4-[[3-[[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-4-(2-furanylcarbonyl)- (9CI) (CA INDEX NAME)



RN 427896-76-2 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(1-methylethoxy)phenyl]- (9CI) (CA INDEX NAME)

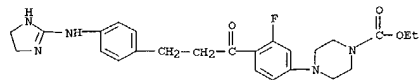


RN 427896-77-3 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(4-methylethoxy)phenyl]- (9CI) (CA INDEX NAME)

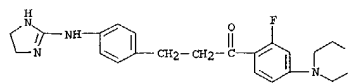


RN 427896-78-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]-3-fluorophenyl]-, ethyl ester (9CI) (CA INDEX NAME)

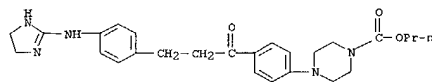
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



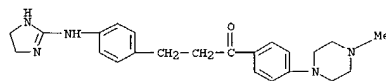
RN 427896-79-5 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[2-fluoro-4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



RN 427896-80-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-, propyl ester (9CI) (CA INDEX NAME)

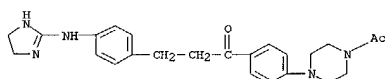


RN 427896-81-9 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(4-methyl-1-piperazinyl)phenyl]- (9CI) (CA INDEX NAME)

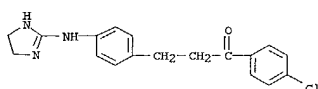


RN 427896-82-0 CAPLUS
CN Piperazine, 1-acetyl-4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]- (9CI) (CA INDEX NAME)

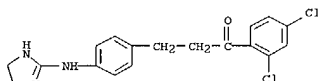
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



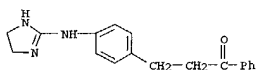
RN 427896-83-1 CAPLUS
CN 1-Propanone, 1-[4-chlorophenyl]-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]- (9CI) (CA INDEX NAME)



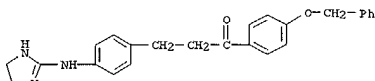
RN 427896-84-2 CAPLUS
CN 1-Propanone, 1-(2,4-dichlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]- (9CI) (CA INDEX NAME)



RN 427896-85-3 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-phenyl- (9CI) (CA INDEX NAME)

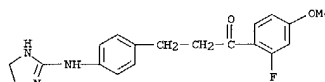


RN 427896-86-4 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



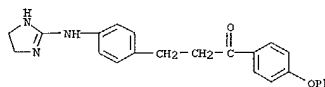
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 427896-87-5 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-fluoro-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 427896-88-6 CAPLUS
CN 1-Propanone, 1-(2,4-dichlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]- (9CI) (CA INDEX NAME)

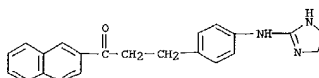
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CRN 427896-88-6
CMF C24 H23 N3 O2



CM 2
CRN 144-62-7
CMF C2 H2 O4

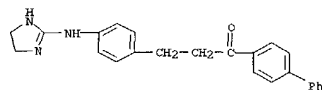


RN 427896-90-0 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

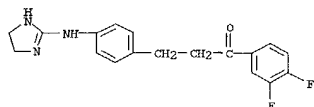


RN 427896-91-1 CAPLUS
CN 1-Propanone, 1-[1,1'-biphenyl]-4-yl-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]- (9CI) (CA INDEX NAME)

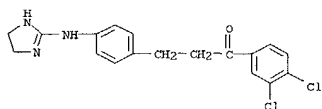
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



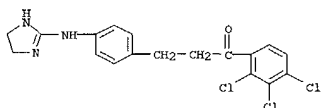
RN 427896-92-2 CAPLUS
CN 1-Propanone, 1-[(3,4-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-fluorophenyl)]- (9CI) (CA INDEX NAME)



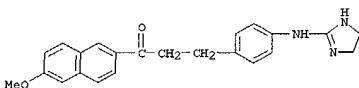
RN 427896-93-3 CAPLUS
CN 1-Propanone, 1-[(3,4-dichlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2,3,4-trichlorophenyl)]- (9CI) (CA INDEX NAME)



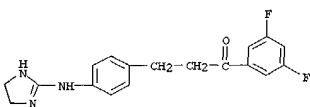
RN 427896-94-4 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2,3,4-trichlorophenyl)- (9CI) (CA INDEX NAME)



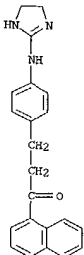
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 427897-00-5 CAPLUS
CN 1-Propanone, 1-[(3,5-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(6-methoxy-2-naphthalenyl)]- (9CI) (CA INDEX NAME)



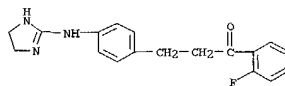
RN 427897-01-6 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(1-naphthalenyl)- (9CI) (CA INDEX NAME)



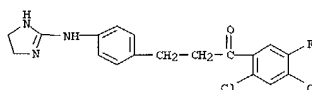
RN 427897-02-7 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(4-fluorophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

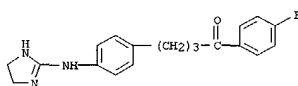
RN 427896-95-5 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-fluorophenyl)- (9CI) (CA INDEX NAME)



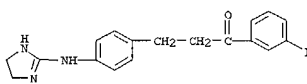
RN 427896-96-6 CAPLUS
CN 1-Propanone, 1-[(2,4-dichloro-5-fluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(4-fluorophenyl)]- (9CI) (CA INDEX NAME)



RN 427896-97-7 CAPLUS
CN 1-Butanone, 4-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

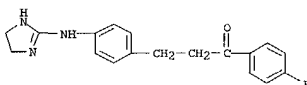


RN 427896-98-8 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(3-fluorophenyl)- (9CI) (CA INDEX NAME)



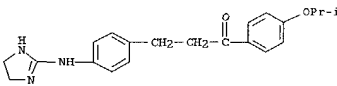
RN 427896-99-9 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



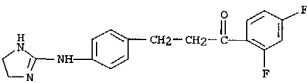
● HCl

RN 427897-03-8 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-[4-(1-methylethoxy)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

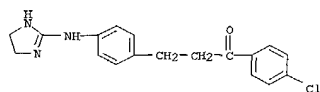
RN 427897-04-9 CAPLUS
CN 1-Propanone, 1-(2,4-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

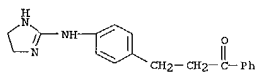
RN 427897-05-0 CAPLUS
CN 1-Propanone, 1-(4-chlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



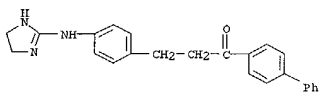
● HCl

RN 427897-06-1 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

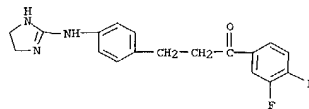
RN 427897-07-2 CAPLUS
CN 1-Propanone, 1-[1,1'-biphenyl]-4-yl-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

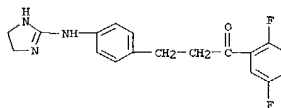
RN 427897-08-3 CAPLUS
CN 1-Propanone, 1-(3,4-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



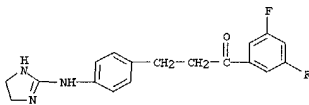
● HCl

RN 427897-09-4 CAPLUS
CN 1-Propanone, 1-(2,5-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

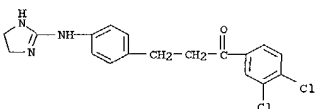
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CN 1-Propanone, 1-(3,5-difluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

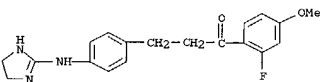
RN 427897-11-8 CAPLUS
CN 1-Propanone, 1-(3,4-dichlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



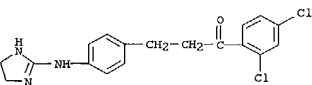
● HCl

RN 427897-12-9 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-fluoro-4-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

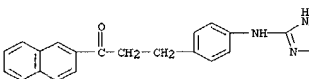
RN 427897-13-0 CAPLUS
CN 1-Propanone, 1-(2,4-dichlorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

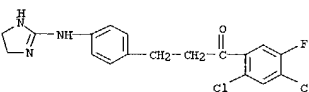
RN 427897-14-1 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



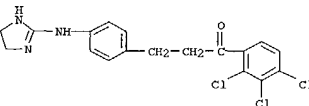
● HCl

RN 427897-15-2 CAPLUS
CN 1-Propanone, 1-(2,4-dichloro-5-fluorophenyl)-3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

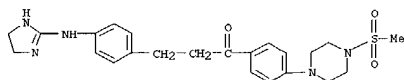
RN 427897-16-3 CAPLUS
CN 1-Propanone, 3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2,3,4-trichlorophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

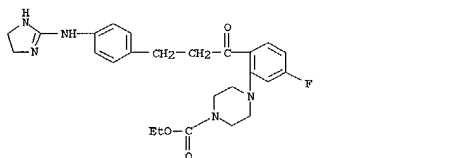
RN 427897-29-8 CAPLUS
CN Piperazine, 1-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(2-oxopropyl)phenyl]-4-(methylsulfonyl)]-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



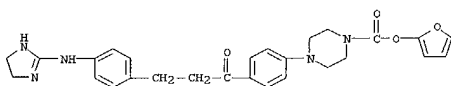
● HCl

RN 427897-30-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]-5-fluorophenyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 427897-31-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-, 2-furanyl ester (9CI) (CA INDEX NAME)



RN 427897-32-3 CAPLUS
CN Piperazine, 1-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]phenyl]-4-(propylsulfonyl)- (9CI) (CA INDEX NAME)

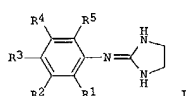
L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:314917 CAPLUS
DOCUMENT NUMBER: 136:325543
TITLE: Preparation of aminophenyliminoimidazolidines for treating urinary incontinence.
INVENTOR(S): Esser, Franz; Pouzet, Pascale; Arielle Jane-Jones; Kitagawa, Hisator; Sakai, Kenji; Muramatsu, Ikunobu
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: PCT Int. Appl., 28 pp.
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032876	A2	20020425	WO 2001-EP11764	20011011
WO 2002032876	A3	20020718		
<p>V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, SV, TH, TJ, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
AU 2002015943	A5	20020429	AU 2002-15943	20011011
DE 10150312	A1	20020704	DE 2001-10150312	20011011
EP 1328517	A2	20030723	EP 2001-987747	20011011
<p>R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR</p>				
EE 200300177	A	20030815	EE 2003-177	20011011
US 2002161031	A1	20021031	US 2001-976917	20011012
US 6602897	B2	20030805		
US 2003158420	A1	20030821	US 2003-349993	20030123
NO 2003001697	A	20030526	NO 2003-1697	20030411
<p>PRIORITY APPLN. INFO.: DE 2000-10051005 A 20001014 US 2000-248172P P 20001114 WO 2001-EP11764 W 20011011 US 2001-976917 A1 20011012</p>				

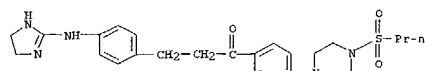
OTHER SOURCE(S): MARPAT 136:325543

GI

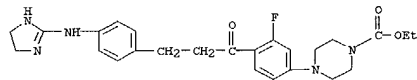


AB Use of title compds. (I; R1 = F, Cl, Br, CH2F, CF2H, CF3; R2 = NR6R7; R6 = Me, Et, Pr, iPr; R7 = Me, Et, Pr, R3, R4, R5 = H, Me, F, Cl, Br, CH2F, CF2H, CF3) for treatment of urinary incontinence, particularly stress incontinence, is claimed. Thus, 2'-bromo-5'-dimethylamino-6'-methylphen-1-yl-2-iminoimidazolidine in H2SO4 at 0.degree. was treated

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

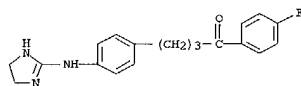


RN 427897-33-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[3-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-oxopropyl]-3-fluorophenyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 427897-36-7 CAPLUS
CN 1-Butanone, 4-[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]phenyl]-1-(4-fluorophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

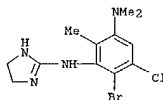
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

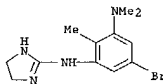
with 1,3-dichloro-5,5-dimethylhydantoin under stirring followed by heating for 3 days at 55.degree. to give 2'-bromo-3'-chloro-5'-dimethylamino-6'-methylphen-1'-yl-2-iminoimidazolidine. The latter as the hydrochloride gave 90% of the activity of noradrenaline in the human urethra.

IT 414868-71-6P 414868-72-7P 414868-73-8P
414868-74-9P
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses)
(prepn. of aminophenyliminoimidazolidines for treating urinary incontinence)

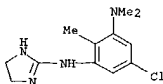
RN 414868-71-6 CAPLUS
CN 1,3-Benzenediamine, 4-bromo-5-chloro-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)



RN 414868-72-7 CAPLUS
CN 1,3-Benzenediamine, 5-bromo-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)



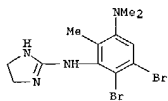
RN 414868-73-8 CAPLUS
CN 1,3-Benzenediamine, 5-chloro-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



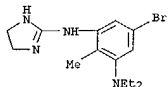
● HCl

RN 414868-74-9 CAPLUS
CN 1,3-Benzenediamine, 4,5-dibromo-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)

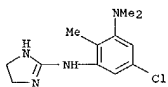
L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 414868-78-3 414868-79-4
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (prepn. of aminophenyliminoimidazolidines for treating urinary incontinence)
 RN 414868-78-3 CAPLUS
 CN 1,3-benzenediamine, 5-bromo-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)



RN 414868-79-4 CAPLUS
 CN 1,3-benzenediamine, 5-chloro-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)



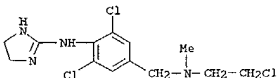
IT 183555-51-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aminophenyliminoimidazolidines for treating urinary incontinence)
 RN 183555-51-3 CAPLUS
 CN 1,3-benzenediamine, 4-bromo-N3-(4,5-dihydro-1H-imidazol-2-yl)-N1,N1,2-trimethyl- (9CI) (CA INDEX NAME)

L9 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

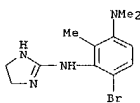
ACCESSION NUMBER: 1997:571348 CAPLUS
 DOCUMENT NUMBER: 127:229940
 TITLE: Alpha1-adrenergic receptor subtypes in the urinary tract of the rat
 AUTHOR(S): Miranda, H. P.; Maquie, D.; Pinardi, G.
 CORPORATE SOURCE: Faculty Medicine, Universidad Chile, Santiago, Chile
 SOURCE: Pharmacology Reviews and Communications (1997), 9(3), 197-204
 CODEN: PHRCF6
 PUBLISHER: Harwood
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The .alpha.1-adrenergic receptor subtypes were identified involved in contraction of the urinary bladder, prostate, and vas deferens of the rat, using 5-methylurapidil (5-MU) and chloroethylclonidine (CEC) as subtype-selective antagonists. Administration of norepinephrine (NE) and phenylephrine (PHE) produced dose-dependent contractions of all tissues, with different EC50's and Emax. 5-MU (1-100 nM) produced parallel shifts to the right of the control NE and PHE dose-response curves, without changes in Emax. Pretreatment with CEC (30 or 50 .mu.M) inhibited the response to NE and PHE in the prostatic portion of the vas deferens and in the prostate but did not modify the response in the epididymal segment of the vas deferens or in the urinary bladder. According to the rank order of agonist potency and the selectivity of 5-MU and CEC, these results suggest that contraction of rat urinary bladder, vas deferens, and prostate are mediated primarily by the .alpha.1A-subtype, however with some contribution of the .alpha.1B-subtype in the prostatic segment of vas deferens and the prostate.

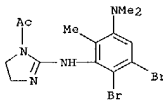
IT 77472-95-8, Chloroethylclonidine
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (effect on urinary bladder contractions to norepinephrine and phenylephrine)
 RN 77472-95-8 CAPLUS
 CN 1H-imidazol-2-amine, N-[2,6-dichloro-4-[(2-chloroethyl)methylamino]methyl]phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 414868-86-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of aminophenyliminoimidazolidines for treating urinary incontinence)
 RN 414868-86-3 CAPLUS
 CN 1H-imidazol-2-amine, 1-acetyl-N-[2,3-dibromo-5-(dimethylamino)-6-methylphenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



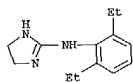
L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:318325 CAPLUS
 DOCUMENT NUMBER: 127:13229
 TITLE: The peripheral action of clonidine analog ST-91: involvement of atrial natriuretic factor
 AUTHOR(S): Gutkowska, Jolanta; Mukaddam-Daher, Suhayla; Tremblay, Johanne
 CORPORATE SOURCE: Laboratory Cardiovascular Biochemistry, Centre Recherche Hotel-Dieu Montreal, Universite Montreal, Montreal, QC, H2W 1T8, Can.
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (1997), 281(2), 670-676
 CODEN: JPETAB; ISSN: 0022-3565
 PUBLISHER: Williams & Wilkins
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB It is generally thought that the cardiovascular and renal effects of clonidine, an alpha-2 adrenergic agonist, are mediated by central mechanisms. Our previous work has shown that diuresis and natriuresis caused by central administration of clonidine are mediated by an enhanced release of atrial natriuretic factor (ANF). Because clonidine has been shown to have peripheral actions the objective of the present study was to det. whether ANF is also involved in these actions. Studies were performed with use of a structural clonidine analog, ST-91, which does not cross the blood-brain barrier. I.v. injection of various doses (0-250 .mu.g/rat) of ST-91 into conscious, normally hydrated female Sprague-Dawley rats (200-250 g) produced dose-related increases in urinary output, which were accompanied by significant increases in urinary sodium, potassium and cGMP excretion. Compared with saline, the highest dose of ST-91 (250 .mu.g/rat) during the first hour of treatment significantly (P < .001, n = 18) enhanced urinary output (0.2 +/- 0.1 vs. 3.0 +/- 1.1 mL/h) and excretion of sodium (28 +/- 4 vs. 345 +/- 50 .mu.mol/h), potassium (10 +/- 4 vs. 165 +/- 37 .mu.mol/h) and cGMP (191 +/- 29 vs. 1340 +/- 322 pmol/h), the biol. marker of ANF. These renal responses were assoc. with increased plasma ANF (59 +/- 28 pg/mL, P < .001, n = 12), measured 10 min after ST-91 (250 .mu.g/rat), which remained elevated for at least 1 h (P < .01, n = 6). The enhanced renal responses that were induced by 10 .mu.g ST-91 were partially, yet significantly inhibited by yohimbine (50 .mu.g), an alpha-2 antagonist. On the other hand, efaroxan (500 .mu.g), an 11 imidazoline receptor antagonist, showed a stronger inhibitory effect, whereas naloxone (0.8 mg) had no effect. Pretreatment of rats with anti-ANF reduced the diuretic and natriuretic effects of ST-91. These results indicate that the renal effects of ST-91 are mediated by imidazoline as well as by alpha-2 adrenergic receptors, but not by opioid receptors. Furthermore, the renal effects evoked by ST-91 are mediated by ANF.

IT RL: PAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (peripheral action of clonidine analog ST-91: involvement of atrial natriuretic factor)
 RN 4749-61-5 CAPLUS
 CN 1H-imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:1110 CAPLUS
 DOCUMENT NUMBER: 112:1110
 TITLE: .alpha.2-Adrenergic receptors and the sodium/hydrogen ion exchanger in the intestinal epithelial cell line, HT-29

AUTHOR(S): Cantiello, Horacio F.; Lanier, Stephen M.
 CORPORATE SOURCE: Massachusetts Gen. Hosp., Harvard Med. Sch., Boston, MA, 02114, USA
 SOURCE: Journal of Biological Chemistry (1989), 264(27), 16000-7

CODEN: JBCHA3; ISSN: 0021-9258
 DOCUMENT TYPE: Journal

LANGUAGE: English
 AB The effect of .alpha.2-adrenergic receptors (.alpha.2-AR) activation on

basal and stimulated Na⁺/H⁺ exchange was studied in epithelial cells isolated from human colon (HT-29 adenocarcinoma cells). Na⁺/H⁺ exchange was measured by quantitation of intracellular H⁺ ion concn. (acetoxymethyl ester 2,7-biscarboxyethyl-5(6)carboxyfluorescein) and 22Na⁺ uptake. HT-29 cells expressed an amiloride-sensitive Na⁺/H⁺ exchanger that was activated by redn. of intracellular pH (pHi) to 6.0 but was quiescent at a physiol. pHi. The rapid alkalinization obsd. after acid loading (0.57 pH units/min/104 cells) was dependent on external Na and was blocked by amiloride (Ki .apprx.2.1 .mu.M). Although epinephrine and the selective .alpha.2-AR agonists clonidine and UK-14304 inhibited forskolin-activated adenylyl cyclase, these compds. did not alter basal Na⁺/H⁺ exchange. Stimulated Na⁺/H⁺ exchange was similarly unaffected by epinephrine. In contrast, stimulated Na⁺/H⁺ exchanger activity was completely inhibited by the selective .alpha.2-agonists clonidine, UK-14304, and guanabenz. This inhibitory effect was not blocked by the .alpha.2-AR antagonist rauwolfscine, and it is likely due to a direct interaction with the exchanger mol. itself. Structure/activity studies indicated that the compds. inhibiting exchanger activity possess either an imidazoline or guanidinium moiety. Although these mols. bear structural similarity to amiloride, they did not inhibit the amiloride-sensitive epithelial Na channel in toad urinary bladder, suggesting that these compds. may be useful as amiloride-like ligands selective for the Na⁺/H⁺ exchanger. Evidently, in the HT-29 intestinal cell line, in contrast to observations in other tissues, .alpha.2-AR are not coupled to the Na⁺/H⁺ exchanger, suggesting that the cell-signaling mechanisms utilized by the .alpha.2-AR are tissue specific.

IT 4749-61-5, ST-91 77472-95-8, Chloroethylclonidine

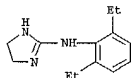
RL: BIOL (Biological study)

(hydrogen ion-sodium exchange transport inhibition by, in intestine epithelial cells of human, structure in relation to)

RN 4749-61-5 CAPLUS

CN 1H-imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

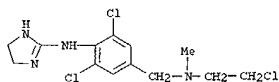
L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

RN 77472-95-8 CAPLUS

CN 1H-imidazol-2-amine, N-[2,6-dichloro-4-[(2-chloroethyl)methylamino]methyl]phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 06:55:50 ON 09 OCT 2003)

FILE 'REGISTRY' ENTERED AT 06:55:57 ON 09 OCT 2003

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 23 S L2 FULL

FILE 'CAPLUS' ENTERED AT 06:56:50 ON 09 OCT 2003

L4 18 S L3

FILE 'REGISTRY' ENTERED AT 07:01:56 ON 09 OCT 2003

L5 STRUCTURE UPLOADED
L6 1145 S L5 FULL

FILE 'CAPLUS' ENTERED AT 07:02:20 ON 09 OCT 2003

L7 621 S L6
L8 603 S L6 NOT L4
L9 5 S L8 AND URINARY

=> s l8 and adrenergic

70117 ADRENERGIC
260 ADRENERGICS
70165 ADRENERGIC
(ADRENERGIC OR ADRENERGICS)

L10 243 L8 AND ADRENERGIC

=> s l10 and alpha

1437720 ALPHA
2483 ALPHAS
1437815 ALPHA
(ALPHA OR ALPHAS)

L11 238 L10 AND ALPHA

=> s l11 and agonist

89685 AGONIST
66678 AGONISTS
122766 AGONIST
(AGONIST OR AGONISTS)

L12 148 L11 AND AGONIST

=> s l12 andphenyliminoimidazolidine

MISSING OPERATOR L12 ANDPHENYLIM

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l12 and phenyliminoimidazolidine

26 PHENYLIMINOIMIDAZOLIDINE
28 PHENYLIMINOIMIDAZOLIDINES
46 PHENYLIMINOIMIDAZOLIDINE
(PHENYLIMINOIMIDAZOLIDINE OR PHENYLIMINOIMIDAZOLIDINES)

L13 4 L12 AND PHENYLIMINOIMIDAZOLIDINE

=> d ibib abs hitstr 1-4

L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:468606 CAPLUS

DOCUMENT NUMBER: 119:68606

TITLE: Biochemical and physiological effects of octopamine and selected octopamine agonists on the oviducts of Locusta migratoria

AUTHOR(S): Lange, Angela B.; Tsang, Peter K. C.

CORPORATE SOURCE: Dep. Zool., Univ. Toronto, Mississauga, ON, L5L 1C6, Can.

SOURCE: Journal of Insect Physiology (1993), 39(5), 393-400

CODEN: JIPHAF; ISSN: 0022-1910

DOCUMENT TYPE: Journal

LANGUAGE: English

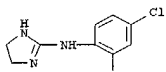
AB The effects of octopamine and some selected octopamine agonists on neurally-evoked contractions and cAMP levels of the lateral oviducts of the locust, *L. migratoria*, were examd. Octopamine caused reversible, dose-dependent decreases in both the basal tonus and amplitude of neurally-evoked contractions of the lateral oviducts, and inhibited myogenic contractions. The 2-aminooxazoline, AC6 [2-(4-chloro-*o*-toluidino)-2-oxazoline], and the substituted phenyliminoimidazolidines (PIIs), NC5 (2,6-diethyl-Pii) and NC7 (2-methyl-4-chloro-Pii), were each capable of eliciting similar responses to octopamine on neurally-evoked contractions. The vertebrate .alpha.-adrenergic receptor antagonist phentolamine blocked the physiol. effects of all agonists tested. The effect of these agonists on cAMP levels was also examd. Octopamine and the 3 agonists were able to increase the cAMP content of the lateral oviducts in a dose-dependent manner. The increases in cAMP were inhibited in the presence of various vertebrate receptor antagonists. The results of this study indicate that AC6, NC5, and NC7 all act as agonists to the octopamine2-like receptors present on locust oviduct and confirm previous studies for the agonistic properties of these agents.

IT 4201-26-7, NC 7 4751-48-8, NC 5

RL: BIOL (Biological study)
(oviduct cAMP and contraction response to, in locust)

RN 4201-26-7 CAPLUS

CN 1H-Imidazol-2-amine, N-(4-chloro-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 4751-48-8 CAPLUS

CN 1H-Imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:144798 CAPLUS

DOCUMENT NUMBER: 102:144798

TITLE: Characterization of octopamine-sensitive adenylate cyclase: elucidation of a class of potent and selective octopamine-2 receptor agonists with toxic effects in insects

AUTHOR(S): Nathanson, James A.

CORPORATE SOURCE: Dep. Neurol., Harvard Med. Sch., Boston, MA, 02114, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1985), 82(2), 599-603

CODEN: PNASAG; ISSN: 0027-8424

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Octopamine [104-14-3]-2 receptors, assocd. with activation of adenylate cyclase [9012-42-4], mediate a no. of the important hormonal and neurotransmitter functions of octopamine in invertebrates. By utilizing the highly enriched octopamine-sensitive adenylate cyclase present in the firefly light organ, it was possible to characterize octopamine-2 receptors pharmacol. and to define a new class of highly potent and selective octopamine-2 agonists. At low concns., these substituted phenyliminoimidazolidines stimulate light emission when injected into fireflies. At somewhat higher concns., these compds., when ingested by tobacco hornworms, cause disruption of motor and feeding behavior, leading to insect death. The effects of these compds. are markedly potentiated by phosphodiesterase inhibitors and mimicked by other activators of octopamine-sensitive adenylate cyclase, including octopamine itself. Because octopamine-2 receptors appear to be present primarily in invertebrates, these findings, together with other data, raise the possibility that potent and selective octopamine agonists could be useful as insect toxins with low toxicity in vertebrates.

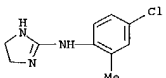
IT 4201-26-7 4201-40-5 4751-48-8

4794-83-6 16822-94-9

RL: BIOL (Biological study)
(octopamine-sensitive adenylate cyclase of firefly activation by, kinetics of)

RN 4201-26-7 CAPLUS

CN 1H-Imidazol-2-amine, N-(4-chloro-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

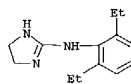


RN 4201-40-5 CAPLUS

CN 1H-Imidazol-2-amine, 4,5-dihydro-N-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

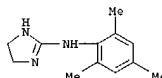
L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

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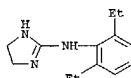
L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

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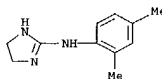
RN 4751-48-8 CAPLUS

CN 1H-Imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



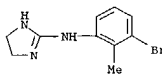
RN 4794-83-6 CAPLUS

CN 1H-Imidazol-2-amine, N-(2,4-dimethylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

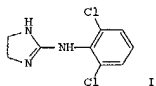


RN 16822-94-9 CAPLUS

CN 1H-Imidazol-2-amine, N-(3-bromo-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



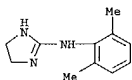
L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1983:551726 CAPLUS
 DOCUMENT NUMBER: 99:151726
 TITLE: Quantitative structure-activity relationships of imidazolidine derivatives related to clonidine at peripheral .alpha.-adrenoceptors
 AUTHOR(S): Medgett, I. C.; McCulloch, M. W.
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Melbourne, Parkville, 3052, Australia
 SOURCE: Clinical and Experimental Pharmacology and Physiology (1983), 10(4), 395-410
 CODEN: CEXPB9; ISSN: 0305-1870
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



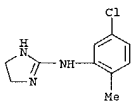
AB The effects of clonidine (I) [4205-90-7], oxymetazoline [1491-59-4] and 13 substituted phenyliminoimidazolidine analogs of clonidine were studied and compared on postjunctional .alpha.-adrenoceptors in guinea pig and rabbit aorta and on prejunctional .alpha.-adrenoceptors in guinea pig atria. In the aorta, all compds. were partial agonists at postjunctional .alpha.-adrenoceptors. Correlation of agonist potency with various combinations of their physicochem. parameters alone detd. 92% of the variance in the data with potency being primarily and highly correlated with pKa. Similarly, in atria, all compds., with the possible exceptions of St 95 [4059-06-7] and St 1943 [57101-49-2], appeared to be partial agonists at prejunctional .alpha.-adrenoceptors; transmitter noradrenaline [51-41-2] release could either be inhibited (field stimulation at 1 Hz for 5 s) or enhanced (5 Hz for 30 s). Apparently, 2,6-substitution in the Ph ring appears to be a specific non-physicochem. activity-enhancing factor at prejunctional but not postjunctional .alpha.-adrenoceptors. A comparison with data in the literature giving the acute hypotensive potencies of the compds. suggests that central .alpha.-adrenoceptors may more closely resemble atrial prejunctional .alpha.-adrenoceptors than aortic postjunctional .alpha.-adrenoceptors. Quant. correlations between centrally-mediated hypotensive and peripheral vasoconstrictor effects of clonidine-like imidazolidines do not provide a sufficiently sensitive method of distinguishing between .alpha.-adrenoceptor subtypes.

IT 4201-22-3 4201-41-6 4749-61-5
 4059-06-7 16884-24-5 28125-87-3
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

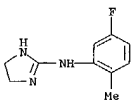


RN 16884-24-5 CAPLUS
 CN 1H-imidazol-2-amine, N-(5-chloro-2-methylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

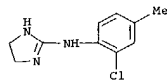


● HCl

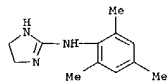
RN 28125-87-3 CAPLUS
 CN 1H-imidazol-2-amine, N-(5-fluoro-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 (.alpha.-adrenoceptor agonist activity of, physicochem. properties and structure in relation to)
 RN 4201-22-3 CAPLUS
 CN 1H-imidazol-2-amine, N-(2-chloro-4-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

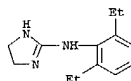


RN 4201-41-6 CAPLUS
 CN 1H-imidazol-2-amine, 4,5-dihydro-N-(2,4,6-trimethylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 4749-61-5 CAPLUS
 CN 1H-imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



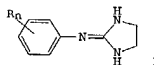
● HCl

RN 4859-06-7 CAPLUS
 CN 1H-imidazol-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1982:607764 CAPLUS
 DOCUMENT NUMBER: 97:207764
 TITLE: Quantitative aspects of alpha adrenergic effects induced by clonidine-like imidazolidines. I. Central hypotensive and peripheral hypertensive activities
 AUTHOR(S): De Jonge, A.; Timmermans, P. B. M. W. M.; Van Zwieten, P. A.
 CORPORATE SOURCE: Div. Pharmacother., Univ. Amsterdam, Amsterdam, Neth.
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (1982), 222(3), 705-11
 CODEN: JPETAB; ISSN: 0022-3565
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Twenty disubstituted and two trisubstituted (phenylimino)imidazolidines I (Rn = F, Br, Cl, OMe, etc.; n = 2 or 3), including clonidine (I; R2 = Cl-2, Cl-6) [4205-90-7] were evaluated for their central hypotensive activity after i.v. administration to anesthetized normotensive rats and peripheral hypertensive activity after i.v. administration to pithed normotensive rats. The partition coeff. (log P') between octanol and aq. buffer (pH 7.4, 37.degree.C) was employed as a measure of the ability of the compds. to penetrate into the central nervous system. Within pairs of 3- and 5-substituted analogs, which are isolipophilic, comparable hypertensive potencies were detd., whereas great differences in hypotensive potencies were found. Hypotensive activity of the 5-substituted mols. always were less pronounced than that of their corresponding 3-substituted isomers. As a consequence thereof, hypo- and hypertensive activities were not correlated within this series of clonidine-like imidazolidines. This outcome contrasts to the results of all correlation studies reported previously. Linear regression anal. showed that hypotensive activity was satisfactorily described by the steric dimensions of the 5-substituent and significantly further improved by inclusion of log P'. Apparently, the presence of a bulky substituent at position 5 of the Ph ring of clonidine-like imidazolidines imparts upon these agonists the ability to discriminate between central hypotensive activity mediated by .alpha.-2-adrenoceptors and peripheral hypertensive potency mediated by .alpha.-1 and .alpha.-2 adrenoceptors. The discrepancy is explained by a distinct structural difference between .alpha.-1 and .alpha.-2 adrenoceptors governed by the allowance for steric bulk at position 5 of (phenylimino)imidazolidines. It is proposed that significant activities always will be ascribed for nonselective agonists of .alpha.-1 and .alpha.-2 adrenoceptors, provided that they possess sufficient lipophilicity to reach the central nervous system. On the other hand, preferentially .alpha.-1 adrenoceptor agonists, e.g., 5-substituted imidazolidines, will not fit into such a relationship due to their enhanced pressor/depressor ratio.

IT 16822-80-3 16822-85-5 16822-85-9
 16822-94-9 16822-97-2 28125-87-3

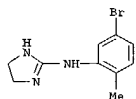
L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

82801-84-1 83690-78-2

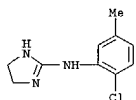
RL: BIOL (Biological study)

(central hypotensive and peripheral hypertensive activities of, .alpha.-adrenoceptor populations in, lipophilicity in relation to)

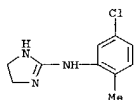
RN 16822-80-3 CAPLUS
CN 1H-Imidazol-2-amine, N-(5-bromo-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 16822-82-5 CAPLUS
CN 1H-Imidazol-2-amine, N-(2-chloro-5-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

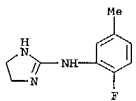


RN 16822-85-8 CAPLUS
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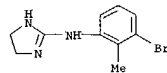


RN 16822-94-9 CAPLUS
CN 1H-Imidazol-2-amine, N-(3-bromo-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

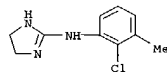
L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



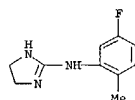
L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



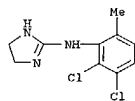
RN 16822-97-2 CAPLUS
CN 1H-Imidazol-2-amine, N-(2-chloro-3-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 28125-87-3 CAPLUS
CN 1H-Imidazol-2-amine, N-(5-fluoro-2-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 82801-84-1 CAPLUS
CN 1H-Imidazol-2-amine, N-(2,3-dichloro-6-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 83690-78-2 CAPLUS
CN 1H-Imidazol-2-amine, N-(2-fluoro-5-methylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

52.77

434.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-5.86

-17.58

STN INTERNATIONAL LOGOFF AT 07:07:13 ON 09 OCT 2003